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Structure, scale and emergence

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ABSTRACT

In this paper I consider the structures that chemists and physicists attribute at the molecular scale to substances and materials of various kinds, and how they relate to structures and processes at other scales. I argue that the structure of a substance is the set of properties and relations which are preserved across all the conditions in which it can be said to exist. In short, structure is abstraction. On the basis of this view, and using concrete examples, I argue that structures, and therefore the chemical substances and other materials to which they are essential, are emergent. Firstly, structures themselves are scale-dependent because they can only exist within certain physical conditions, and a single substance may have different structures at different scales (of length, time and energy). Secondly, the *distinctness* of both substances and structures is a scale-dependent relationship: above a certain point, two distinct possibilities may become one. Thirdly, the necessary conditions for composition, for both substances and molecular species, are scale-dependent. To know whether a group of nuclei and electrons form a molecule it is not enough to consider energy alone: one also has to know about their environment and the lifetime over which the group robustly hangs together.

1. How not to think about composition and structure

Philosophers are apt to fall into three kinds of trap when thinking about structure and composition, and how the reality we find at different scales all fits together. One is to assume that it is helpful to think about the molecular world in precisely the same terms as macroscopic inanimate objects. A second is to assume that the macroscopic world is so unlike the everyday world that nothing of any metaphysical substance can be said about molecular reality. All bets are off 'down there'. A third is to embrace the strangeness, even revelling in it and ignoring the genuine knowledge that science gives us of what goes on at larger scales.[1]

Philosophers fall into the first kind of trap when they hear talk of 'microstructures'—physical relationships between nuclei and electrons at the molecular scale—and assume that these microstructures resemble the things called 'arrangements' into which they are able to place macroscopic inanimate objects. This is misleading in a number of ways. Firstly, 'arrangement' suggests something static, whereas nuclei and electrons are constantly in motion. In fact if quantum mechanics is correct it is (at least nomologically) impossible for them to be entirely at rest. This has important consequences for what we should understand by the word 'structure'. Secondly, taking 'arrangements' of macroscopic inanimate objects as the model for thinking about how atoms or subatomic particles form larger structures assumes that they aggregate and form (or fail to form) composite objects in just the same ways as bricks or billiard balls. This is surely false, because there are principled (nomic or metaphysical) reasons why, for instance, we cannot recover an atom from a molecule in the way that we can (in principle) recover a particular brick from a demolished house. Thirdly, 'arrangement' invokes a purely spatial relationship between parts, but this entirely neglects two physical quantities that are central to understanding structure and composition in the material sciences: energy and time. Lastly, 'arrangement' suggests frailty and fragility (or at least allows it), while the structure of a molecule is robust: there are internal forces holding it

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[1] In their manifesto for a naturalist metaphysics, James Ladyman, Don Ross, David Spurrett and John Collier (2007) identify and avoid the first and second of these traps. I am less sure about the third one. Although I am sympathetic to the idea that there is an asymmetrical relationship between physics and special sciences, their 'Principle of Naturalistic Closure' (2007, 37) and 'Primacy of Physics Constraint' (2007, 38) give too much privilege to what they call 'fundamental' physics, and in quite the wrong way. I fear that these two principles lead them to take too seriously some non-representative mathematical features of physical theories whose acceptance is temporary.

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together, which means that it can survive some motion among its parts, and some distortion by external forces. Such an object is more than just an arrangement.[2]

Other philosophers avoid the first trap, realising that the everyday world might not always be a good guide to understanding the molecular world, and acknowledging (even embracing) its Heraclitean strangeness. But they fall into another trap when they become *too* impressed by this. Arthur Eddington must take some of the blame, when he distinguished between the commonsense and scientific conceptions of the table on which he was writing (1928, xi-x). The former is solid and substantial, while the latter is insubstantial, consisting mostly of empty space. According to science 'the paper before me is poised as it were on a swarm of flies and sustained in shuttlecock fashion by a series of tiny blows from the swarm underneath' (1928, x). Eddington thought there was strong scientific evidence for the emptiness he invoked: Ernest Rutherford had argued that the behaviour of α-particles fired through thin gold foil showed that most of the mass and charge was concentrated in a volume which is very small compared with the size of the gold atoms (Eddington, 1928, pp. 1–2). What had appeared to be a solid material now turned out to be just so much empty space! Eddington can be forgiven his error on the grounds that he was writing early in the development of quantum theory, before its insights had properly been integrated into the physics of materials. Unfortunately his discussion of the two tables has encouraged many philosophers to paint the same verbal pictures, often buzzing with insect metaphors. W.V. Quine asked of the molecular theory: 'Does it repudiate our familiar solids and declare for swarms of molecules, or does it keep the solids and explain them as subvisibly swarming with molecules?' (1960, 265). In contrasting the manifest and the scientific image, Wilfrid Sellars also cited Eddington, claiming that theoretical physics (1991, 35–6) viewed 'man' as a 'swirl of physical particles, forces, and fields' (1991, 20). More recently, David Lewis assumed that 'all things are swarms of particles' (1999, 164), while according to Achille Varzi 'material objects are just swarms of subatomic particles frantically dancing in an otherwise empty space' (2011, 136).

These are deeply misleading pictures. Matter is far from being empty space. An atom fills the space it occupies, and it does so by being partly composed of bound electrons that exclude the bound electrons of which other atoms are partly composed. On most interpretations of quantum mechanics, electrons are not like the golden snitch of quidditch, flitting about here and there but always being somewhere, allowing the α-particles to lumber through unimpeded (like bludgers, but without always causing the same havoc). For the purposes of understanding the collective properties of nuclei and electrons in matter at the macroscopic scale, the electron is smeared out across all of the space occupied by the atom, unless something physical is done to localise it. Eddington's inference to emptiness is also mistaken because it treats solidity as an all-or-nothing affair. Solidity is more like hardness, in that an object is solid to the degree that it can exclude other matter from the space it occupies. Seeing atoms as so much empty space, because one can sometimes fire α-particles though them, is then like saying that diamonds are soft because there exist harder materials that can be used to scratch them. No: Eddington's discussion of his two tables is fatally flawed by its failure to acknowledge that hardness and solidity are scale-relative. Eddington's table is solid at the macroscopic scale, and this is explained by the way its constituent atoms are bonded together and exclude other atoms. Furthermore, the talk of 'swarms' suggests chaos, obscuring the fact that there can be systematic regularities in the motions of particles at the molecular scale, like the orbit of a planet. Of course subatomic particles do not have paths, and so do not have orbits, but there are constants to their motion. It is to the constants of particular motions that chemistry and physics will look for structural explanation at the molecular scale. Given the inferences that philosophers typically draw using the term, one must assume that a 'swarm' is something very complex, with vague boundaries, which is (in a loose sense) composed of much smaller objects. To echo an earlier point, this picture neglects time and energy.

Just as disastrous, in my view, is the third trap, fallen into by philosophers and scientists who are so impressed by the strangeness of the sub-molecular world that they embrace world views which are literally incredible, according to which macroscopic reality as we perceive it is an illusion. Eddington is urged to relinquish his macroscopic table entirely, on the grounds that it embodies folk-intuition rather than scientific knowledge. Only the most fundamental and general principles of physics can say anything worthwhile about physical reality, and so much the worse for anything which isn't deducible from such principles without idealisation or approximation. Or perhaps the evidence of our own eyes is dismissed because we are taken to have only a limited perceptual perspective on reality, either because (i) we can perceive just three dimensions, when according to quantum mechanics we live in a space with many more dimensions, or (ii) we have experiential access only to a single universe, but in reality inhabit a continuously branching multiverse, whose existence can be inferred only by interpreting the mathematical structure of quantum mechanics in just the right way. The mistake here is to pay too much interpretative attention to the *axioms* of the general theory, while ignoring its applications. If a physical theory such as quantum mechanics gives us knowledge of the world, then surely the most secure knowledge it gives us is embodied in its explanatory applications. Philosophers of good sense and good taste would do well to concentrate their attention on these applications, rather than on the axioms of the theory.

Now this paper isn't about tables, or any other 'ordinary' macroscopic objects. It's about chemical substances and molecules. What follows is part of an attempt to understand one aspect of the thinking, workings and results of the material sciences, taking into account the more general perspective of the framework of theories within which, for well over a century, material scientists have taken themselves to be working. I want to explore a conception of structure and composition that is inspired by, and consistent with: (i) the theories, and the classificatory and explanatory practice of the sciences of matter; (ii) the fact that the molecular world is never at rest, so that talk of 'arrangements' is best avoided; (iii) the fact that chemists and physicists sometimes attribute different kinds of structure to the same thing, sometimes at different scales, and that there is no simple rule that one of these must always be prior to the others. My account of structure and composition is therefore in the spirit of the 'scale-free universe' sketched by Mariam Thalos, in which 'there is all manner of activity in the universe, happening at every scale' (2013, 5). It also has much in common with the 'scale relativity of ontology' urged by Ladyman et al. (2007, 199–200).[3] One scale (shorter length or timescales, higher energy) should not be assumed to have priority over the others. I would not deny that we can sometimes argue for the ontological priority of one scale over another, but any such priority has to be earned through specific arguments, grounded in science.

2. Structures in chemistry and physics

Structure at the molecular scale is central to understanding how materials behave. Chemical substances are named for their structures:

[2] For a very clear illustration of the dangers of reasoning about mereological composition in terms of 'arrangements' see Theodore Sider's discussion (2001, Section 4.9).

[3] With two provisos. One I mentioned earlier; a second is that the phrase 'scale-relativity of ontology' suggests Carnap's formal mode: a meta-metaphysical claim that different 'ontologies' can be usefully applied at different scales. 'Scale-relativity of existence' would be more a more congenial way to convey the material-mode (and straightforwardly realist) claim about structure that I am trying to get at.

atoms, ions and the structural relationships between them provide the sole basis for the International Union of Pure and Applied Chemistry's three systems of systematic nomenclature (see Leigh, Favre, & Metanomski, 1998). The structure of substances provides the basis for understanding how they do what they do: reacting with other substances, and transforming into new ones; interacting with radiation and giving rise to their characteristic spectroscopic behaviour, including many of the colours we see around us. This raises a question: just what *is* a structure? In general, the structure of a thing is how its parts fit together to make up the whole. Separating the 'parts' and the 'how', a structure must involve some relata and some relations.[4] As relata, chemical classification and explanation appeals to atoms, ions and (often implicitly) electrons. Things are a little more complicated when it comes to the relations. In other papers (2013, 2016b) I have argued that specifications of structures in chemistry and physics involve two distinct families of relations between atoms, ions and electrons: geometrical relationships and bonds. This generates two distinct but intimately related conceptions of structure, which I have called geometrical structure and bond structure (Hendry, 2013; 2016b). I will now provide a brief account of each, then going on to argue that they are distinct, and that neither kind of structure should be considered more basic than the other.

To ascribe a geometrical structure to a substance or material is to describe stable geometrical relations between its constituent atoms, ions and molecules. A crystal can be described in terms of how its constituent atoms, ions or other groups of atoms are packed together into a three-dimensional lattice. Sodium chloride (NaCl) is composed of positively-charged sodium ions and negatively-charged chloride ions in a one-to-one ratio. *Solid* NaCl is composed of 'two interpenetrating face-centred cubic sub-lattices' (Greenwood, 1968, p. 48), in each of which a sodium (or chloride) ion is surrounded by six chloride (or sodium) ions arranged octahedrally. The crystal may therefore be considered as a (potentially infinite) array of unit cells, each cell containing four sodium ions and four chloride ions (see Fig. 1).

Sodium chloride is a simple example of a crystal, as it is formed by the close-packing of ions which can be regarded as charged spheres, without any internal structure. Other crystalline structures are formed by molecules and ions which do have internal structure: we will discuss them later. The structure of an ionic crystal arises from the close-packing of its ions in a way that minimises the overall energy of the lattice given the charge and relative size of the ions. The force holding the NaCl lattice together is the Coulomb force, which is spherically symmetrical. Hence there are no bonds between the ions, considered as pairwise relationships between the ions: no sodium ion bears any special relationship to any one of its neighbouring chloride ions.

Now a lattice does not consist of *stationary* atoms, molecules or ions:

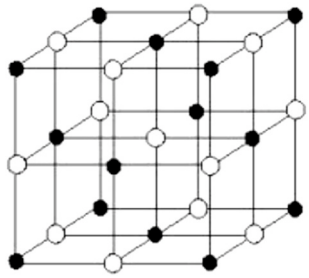

Fig. 1. Solid sodium chloride, after Greenwood, 1968, p. 48.

matter is always in motion, which implies a number of things. Firstly, the lattice structure of salt must involve geometrical relationships between *loci*: small regions of space explored by the ions. Secondly, the higher the temperature the greater the energy available to the ions to explore the space around them, constrained by the lattice. Above a certain temperature (801 °C in the case of NaCl), enough of the ions acquire enough energy to escape the forces holding them in the lattice, which then breaks down, forming a liquid consisting mostly of dissociated ions. Since the ions are now free to move under electrical forces, the molten salt is an electrical conductor, unlike the solid, which is an insulator. Clearly the geometrical structure of solid NaCl does not survive transition to the liquid phase. Since the constituent molecular species in a liquid have far more freedom to move, the structure of a liquid must be characterised in terms of looser spatial relationships between the constituent species: pair correlation functions describing the probability density for given molecular or atomic species in terms of their distance from a specified central atom (see Fig. 2).

Distinct from the purely geometrical structure, which is constituted by spatial relationships between atoms or ions, a substance may have a bond structure (for discussion see Hendry, 2008b, 2013; 2016b): the bond structure of a molecule is the network of bonds connecting its constituent atoms and ions, and which constrains their relative motions. The bond structure of water (a central oxygen atom to which are attached two hydrogens) is not really expressed by the formula 'H_2O', which explicitly conveys only the molar ratio of hydrogen and oxygen in the substance (since no other substance has the formula H_2O, however, it may be used to refer to water without ambiguity). Consider also ethane, C_2H_6: a single bond links two carbon atoms whose remaining valences are used up by six hydrogen atoms. Alternatively, one might say that an ethane molecule consists of two methyl ($-CH_3$) groups connected by a single bond (hence another common formula for ethane is CH_3CH_3). A complete specification of the bond structure of a substance—called a 'full structural formula'—shows every atom and every bond (see Figs. 3 and 4).

Now a full structural formula may or may not provide geometrical information. In Fig. 3, for instance, the angle between the two O–H bonds in the H_2O molecule is shown (approximately) correctly to be around 104°. In Fig. 4 however, the formula for ethane misrepresents the angle between two neighbouring C–H bonds as being around 90°. This is no mistake: the formula is intended to abstract away from any particular geometrical arrangement of the atoms to concentrate on the

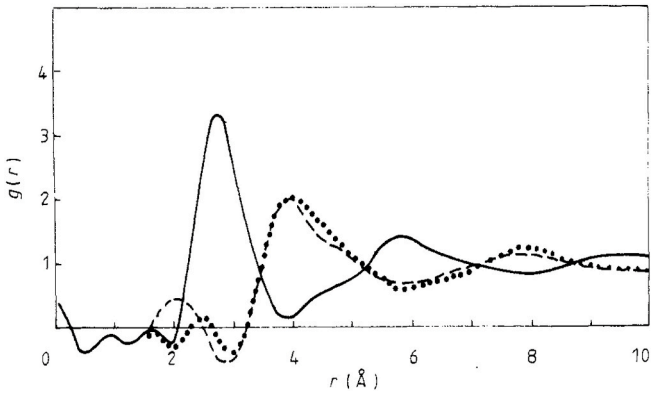

Fig. 2. Pair correlation functions (g(r)) for molten NaCl at 875 °C: solid line g_{NaCl}; dotted line g_{NaNa}; dashed line g_{ClCl}, from Biggin & Enderby, 1982, L306.

connectivity between the atoms. To a large extent this is sufficient to account for ethane's chemical behaviour. In fact, the geometry of the carbon atoms is roughly tetrahedral, the H–C–H angle being around 109°. Further geometrical details of the ethane molecule are complicated by the fact that the two methyl groups rotate quite freely around

[4] Among philosophers, a 'structure' is sometimes taken to involve the relations only, abstracting away from the relata. That is not always how it works in chemistry, where a structure very often includes the relata.

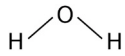

Fig. 3. The full structural formula of water.

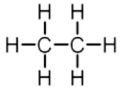

Fig. 4. The full structural formula of ethane.

the single bond between the two carbon atoms. Given the bond angles between the hydrogens attached to each carbon atom,[5] one can distinguish two different geometrical configurations (or *conformations*) that ethane can take: staggered ethane, in which the hydrogen atoms are offset, and eclipsed ethane, in which they are aligned. These two different conformations can be represented in Newman and sawhorse projections, as in Fig. 5.

The staggered conformation is of slightly lower energy than the eclipsed conformation, so rotation around the C–C bond is not entirely free. Nevertheless ethane, as Bassindale colourfully puts it, 'can be thought of in terms of two linked CH_3 propellors, with each CH_3 rotating rapidly' (1984, 25), the eclipsed conformation now appearing as three small regularly occurring hindrances, passed over by the propellors like bumps in the road. Ethane's bond structure, represented in Fig. 4, is an invariant feature through these motions. It is a complex structural property that is shared by all the different conformations.

Geometrical structure and bond structure play independent roles in structural explanation. A simple ionic lattice such as NaCl appears to be constructed without appeal to bonds, at least the localised pairwise relationships between atoms or ions that generate a bond structure. In the case of ethane, the bond structure works as a *constraint* on the geometrical relationships between the molecule's constituent atoms. Bond structure also appears as a constraint on geometrical relationships between atoms within the structures of molecular crystals.[6]

3. Structure, scale and substance

A substance may present distinct structures at different length scales. Seen from afar, a steel bar looks homogeneous, homogeneity being a null kind of structure. Closer in, there are imperfections: discontinuities arising from the grain structure at the millimetre scale. Within the grains are atomic lattices. These differences of structure across scales are reflected in physical explanations of steel's behaviour at the various scales (see Batterman, 2013). A substance may also present distinct structures across different timescales. According to Bassindale 'measurement techniques with relatively long timescales would show an averaged geometry for ethane, but very short-timescale techniques could observe ethane in a staggered conformation' (1984, 51). In the case of ice, Eisenberg and Kauzmann (1969, 150–2) point out that H_2O molecules in ice undergo vibrational, rotational and translational motions, the molecules vibrating much faster than they rotate or move through the lattice. At very short timescales (shorter than the period of vibration), the structure of ice is a snapshot of molecules caught in mid-vibration. It will be disordered because different molecules will be caught at slightly different stages of the vibration. As timescales get longer, the structure averages over the vibrational motions, and then (at yet longer scales) the rotational and translational motions. This yields successively more regular but diffuse structures. Therefore

> the term 'structure' can have three different meanings when applied to a crystal such as ice. The meaning depends on whether one considers a time interval short compared to the period for an oscillation (τ_v), or an interval longer than the period of an oscillation but less than the time for a displacement (τ_D), or an interval considerably longer than the displacement time. (1969, 151).

It may be tempting to assume that the structures presented at close range, and at shorter timescales, are ontologically prior to those observed at longer range and longer timescales. One may even doubt that the longer-range and timescale structures are really distinct at all, if they are just dim impressions of what one would see at close range, or averages over higher-frequency snapshots. In one sense this is correct: if one takes a series of snapshots at a higher frequency, one could reconstruct the average one would see at a lower frequency.[7] Yet there is a counterfactual difference: many different series of snapshots could have given rise to the same average, and which particular series was seen is irrelevant. Put another way, the averaged picture is what one sees at the particular frequency that is appropriate to it. It is not an illusion. These arguments concern timescales. Achille Varzi considers distance, arguing that a boundary seen from afar must be illusory, because it disappears on closer approach:

> It is true that I had the impression of *seeing* the shoreline of Long Island from my plane; but it is also true that when you actually go there, ground-level, things look very different. What looked from the air like a sharp line turns out to be an intricate array of stones, sand, algae, piers, boardwalks, concrete blocks, musk sediments, marshy spots, putrid waters, decayed fish. (2011, 139)

Moreover, if a coastline is identified with the 'water/sand interface' then 'That boundary is constantly in flux, and it is only by filtering it through our cognitive apparatus—it is only by interpolating objects and concepts—that a clear-cut line will emerge.' (2011, 139) I don't think one should dismiss the lower-resolution views. Even if the straightness disappears when one gets closer, a beach that looks long and straight from the air may really present a long straight boundary to incoming water waves, producing plane waves by reflection. Moreover, concentrating only on the view from close up, one may literally lose the bigger picture. The shape of the beach, like the structure of a molecule, depends on the appropriate scale for the process by which one is investigating it. These are matters of physical interaction, not of perception or conception.

A second aspect of the scale-relativity of structure is that relationships of structural sameness and difference vary across different scales. This variation can occur at two different levels: in the way that molecules interact to form macroscopic substances, and in the structural distinctness of the molecules themselves. At the level of the substances, consider Louis Pasteur's achievement in separating, by hand, crystals of the L- and D-forms of sodium ammonium tartrate, obtained from a racemic solution (an equal mixture of the two). This is a famous exemplar of structural explanation in science, and its experimental demonstration, for the L- and D-forms are enantiomers: structures which are mirror images, but which cannot be superimposed on each other. It is less well known that had Pasteur attempted the separation at a higher temperature than he did, he would likely have failed, because above 26 °C the L- and D-salts form a single racemate (Kauffman & Myers, 1975).[8]

For an example of the timescale-dependence of the sameness and difference of molecular structure, consider substituted biphenyls, which

[5] In line with our generally Heraclitean picture there are also regular motions associated with these bond angles. The three hydrogen atoms attached to each carbon wag and vibrate around their central geometry.

[6] See for instance the discussion by Eisenberg and Kauzmann (1969, Chapter 3) of the structure of ice, and Cox, 1958 on benzene. The planarity of the benzene ring was first established crystallographically by Kathleen Lonsdale in the 1920s (Lonsdale, 1929).

[7] My thanks are due to Robert Schoonmaker for raising these points.

[8] My thanks are due to John Hudson for the reference.

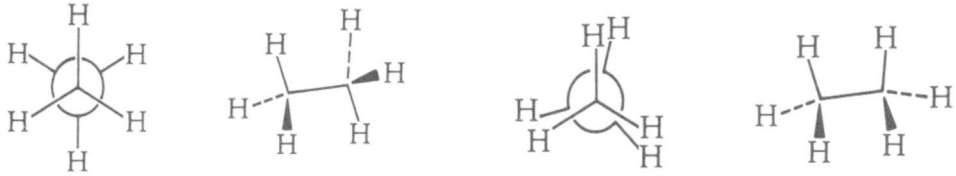

Fig. 5. Newman and sawhorse projections of staggered ethane and eclipsed ethane, from Bassindale, 1984, p. 50.

contain pairs of benzene rings connected by a single bond (see Fig. 6).

When the rings are substituted by functional groups X and Y in the four positions shown, the possibility of a new form of stereoisomerism arises—the molecule can in principle exist in two enantiomeric forms—but the isomerism is interestingly temperature dependent. In general, single carbon-carbon bonds, like the one connecting the two benzene rings, allow free rotation of the groups they connect. If the groups X and Y are relatively small (e.g. single atoms such as hydrogen or fluorine), then that rotation will be relatively unrestricted, though there will be some stearic hindrance: groups X and Y will 'bump' past each other, like the hydrogens in ethane. In such cases the two enantiomers will not be separable at room temperature because they interconvert. There are not two enantiomers, just two enantiomeric conformations of a single structure. For larger X and Y, perhaps the enantiomers can be separated, but they racemize rapidly. For really bulky groups such as $–NO_2$, or –COOH, the interaction between them will constitute a barrier to the rotation, the two enantiomers will be separable and will racemize only slowly. So for any given substituent groups X and Y, the physical distinctness of the enantiomers disappears above a characteristic temperature. Hence structural sameness and difference is a temperature- (and therefore energy-) dependent phenomenon. It also depends on timescale. As Bassindale puts it '*any molecules, of the same molecular constitution, that are rapidly interconverting, at the temperature of measurement are molecules of the same compound*' (1984, 51).

In Section 2, we saw that chemists appeal to two distinct and mutually irreducible kinds of structure: geometrical structure and bond structure. We have just seen that a single substance may have distinct structures at different scales of energy, time and length, and that relationships of sameness and difference between structures vary across different scales. Doesn't that make structure oddly perspectival, or interest-dependent? As long as we understand structure to be a creature of abstraction, there is nothing odd about it at all. A structure is the set of properties and relationships among a substance's parts (at the atomic scale) that remains invariant over the physical conditions under which it exists. It is obtained by abstraction because, from the full array of properties and relations which are present at any particular time, we must subtract those properties and relations that may be present under some conditions and not others. Imagine some chemical substance S within some range of physical conditions C. Let R be the relationships among its parts which survive across C. Over a wider range of physical conditions, some subset of R will be maintained. The strongest structure we can specify for a substance is the set of relationships among its parts that survive across the full range of conditions under which it exists. More can be said about shared structure over narrower ranges of conditions, but we need to find the right level of generality or scale to find commonality among a diverse group of things: right from the point of view of understanding what the substance can do, what it can have done to it, and what it can survive. For the elements, which (modern chemistry assumes) can survive across different states of chemical combination, and even in plasmas, the underlying structures are the nuclei, and in particular their charges. For a compound substance such as water, the abstraction is taken across its different states of aggregation, but all of them are produced by interactions among H_2O molecules. The physical conditions in which water can survive must then be a proper subset of those in which its elemental components can survive: water is dependent on them, and the structures which underwrite their existence.

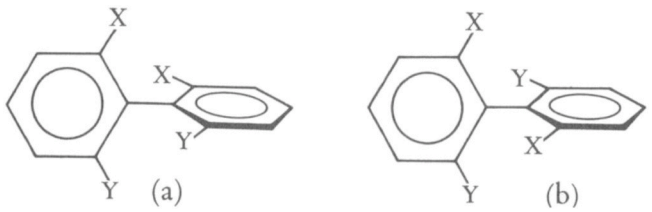

Fig. 6. Biphenyl atropisomers, from Bassindale, 1984, p. 58.

Abstraction is taken to be a form of partial consideration, or selective attention to properties and relation instances existing within a substance across the conditions within which it exists (see Heil, 2003, p. 172). Neither the reality nor the metaphysical seriousness of structure is undermined by this view, for we are selectively attending to such genuine physical properties and relations as charge, mass and spatial proximity. Even chemical bonds can be regarded as topological features of a molecule's electron density distribution (Bader, 1990). (An implication of this is that a chemical bond is a mode: a way for a portion of charge density to be.) These are all genuine properties and relations, rather than mere (monadic or polyadic) predicates, because they are causally efficacious: charges and masses interact via well-known physical laws in ways that depend on spatial proximity, and crystallographers investigate structure by bouncing X-rays off electron density distributions within crystals. It is the *selection* which is interest-dependent, and can be done in different ways, but we are selecting only among the real.

One consequence of this view is that if chemical classification is based on structure, and there is more than one way to abstract away from the structure of a given substance, the a priori requirement that natural schemes of classification should be hierarchical *must* be wrongheaded.[9] One would in general expect just the opposite. Consider NaCl, which shares structural features with diverse groups of substances. Abstracting away from its chlorine content it contains sodium (i.e. nuclei with a charge of 9), which it has in common with (for instance) sodium bromide. Abstracting away from its sodium content it contains chlorine (i.e. nuclei with a charge of 17), which it has in common with potassium chloride and carbon tetrachloride. The sodium-containing substances and the chlorine-containing substances overlap (in sodium chloride), but neither includes the other. Abstracting away from its elemental components entirely, solid sodium chloride is a face-centred cubic crystal, a structure it shares with most of the alkali-metal halides, the alkaline-earth metal oxides and many other ionic substances. Sodium chloride and face-centred cubic crystals overlap, but neither includes the other, for sodium chloride need not be a face-centred cubic crystal (molten sodium chloride is still sodium chloride). In so far as structure underwrites chemical classification, and structure is abstraction, the hierarchy condition must fail (Hendry, 2016a).

There are good reasons to go further than classificatory

[9] According to the hierarchy requirement, no two natural kinds may overlap unless one is contained within the other. For presentation and defence see Ellis, 2001; for criticism see Khalidi, 1998, Tobin, 2010 and Hendry, 2016a. By a 'natural scheme of classification' I mean one whose genera and species are natural kinds.

microstructuralism. Not only does chemistry individuate substances by their structure: perhaps the nature (or essence) of a substance *is* simply its structure. This is not the place to pursue a detailed argument for microstructural essentialism, but here is a sketch of how I think the argument should go. Nancy Cartwright has defended the idea that we can know the (Aristotelian) natures of things through what she calls '*the analytic method* in physics':

> [T]o understand what happens in the world, we take things apart into their fundamental pieces; to control a situation we reassemble the pieces, we reorder them so they will work together to make things happen as we will. You carry the pieces from place to place, assembling them together in new ways and new contexts. But you always assume that they will try to behave in new arrangements[10] as they have tried to behave in others. They will, in each case, act in accordance with their nature. (1992, 49)

Chemical structures are very concrete examples of this. If we wish to employ the powers and susceptibilities of some chemical substance, we must assemble it in the right way from its microstructural parts, or bring it ready made. What is it that carries the powers and susceptibilities of a substance from place to place, or comes into being if we have to assemble it *in situ*? Its structure.[11]

4. Scale and composition

Chemistry concerns itself with at least three kinds of compositional relationship, different in respect of the characteristic scale of the relata. First there are compositional relationships between substances at the macroscopic scale, which have always been central to chemical thought. Lavoisier is credited with establishing that water is a compound of hydrogen and oxygen, and his scientific legacy can be described as a compositional scheme at the base of which are substances, many of which are still recognised as elements by modern chemistry.[12] Second there are compositional relationships between substances and molecular species. These are troubled waters, upon which many confused and confusing discussions of chemical composition and identity have been launched, based on misreadings of the true compositional claim 'water is H_2O'. Third there are compositional relationships between entities at the molecular scale, including nuclei, electrons, atoms and molecules. In what follows I will discuss the first and third kinds of composition in turn. I will not address the second kind of compositional relationship here, except in some brief remarks in the next paragraph (but see Hendry, 2006; 2008a, 2017).

Attempting to discuss 'composition' in chemistry may sound wrongheaded. Perhaps the word 'composition' means different things in chemistry and metaphysics, yielding a pun at best and confusion at worst. I do not think so. Chemistry really is concerned with composition as metaphysicians understand it. I hope my discussion will make that clear. If I am right, 'composition' is unlike 'substance', which means something quite different in metaphysics and in chemistry, though the meanings are clearly related. Chemical substances are kinds of stuff viewed from the perspective of chemistry, a discipline that individuates them by their structure at the molecular scale (or so I argue: see Hendry, 2006). In metaphysics, substances are sometimes taken to be things that do not depend on anything else for their existence or identity, while at other times they are taken to be continuants that can be distinguished from both the properties they bear and the events in which they participate. So long as one can be neutral on the relative priority of continuants and occurrents, I believe that chemical substances meet the latter condition. I do not think they meet the former condition, at least as chemistry conceives of them.[13] I have argued, in this paper and elsewhere (2006, 2008a, 2016a, 2016b), that a chemical substance is the particular substance it is in virtue of certain properties of, and relations between, its constituents at the molecular scale. It follows that it cannot exist without those constituents, and the relevant properties and relations. So chemical substances have a strong kind of existential dependence on their constituents at the molecular scale (namely electrons and nuclei), on their properties, and on relations between them. If substances cannot be dependent on anything else then chemical substances are not substances. So what are they? They must be ways for collections of nuclei and electrons to be: chemical substances are *modes*.[14]

Let us turn to the first kind of compositional relationship, that between chemical substances. Perhaps the oldest foundational question in chemistry, Aristotle's problem of mixture, is how to identify the circumstances in which interaction between two substances, when they are mixed, should be considered as forming a new substance, a chemical combination of the two rather than a mere mixture (see Needham, 2006, 2009).[15] Aristotle argued against survival of the elements in their compounds: the atomist assumption that elements survive precludes a coherent account of chemical combination, he thought, so elements must be 'used up' when they combine. Let us instead follow modern chemistry (and the atomists) and presume the survival of elements in mixtures and compounds. Let us also allow quantities of stuff (some sulphur, or some iron) to count as objects. Under those assumptions, the problem of mixture can be regarded as a specific instance of the Special Composition Question (hereafter SCQ; see van Inwagen 1990): when can it be said, of some group of objects, that it forms a further object? The problem of mixture may not obviously be an instance of the SCQ, but consider the following. A mixture of iron filings and powdered sulphur, and the black crystalline compound ferrous sulphide (iron (II) sulphide, FeS) are easily distinguished: the former is visibly heterogeneous, the latter homogeneous to the eye. Aristotle took homogeneity to be the criterion for when real chemical combination has occurred. Homogeneity excluded the survival of the elements in his view, hence his conclusion that the elements must be 'used up' when genuine combination occurs, but homogeneity in what respects? Homogeneity to the eye is clearly insufficient. Following Aristotle, we may require that as a true compound, every part of iron (II) sulphide is iron (II) sulphide, but

[10] In light of the earlier discussion of misuses of the term 'arrangements,' it is worth pointing out that it is being used here to mean *mode of assembly*, and does not depend on any misleading connotations.

[11] It might seem odd for me to say that THE structure of a substance is essential to it, given that I have just been arguing that substances have different structures at different scales. Which one is the essence? I argued above that structure is abstraction: THE structure of a substance is the set of properties and relations it has whenever it can be said to exist. This allows that a substance might display different structures at different scales, but THE structure is whatever these different structures all have in common. I am most grateful to an anonymous reviewer for raising this point.

[12] Lavoisier is not so often 'credited' with thinking that steam, which we regard as a state of water rather than a distinct substance, has a third component: caloric (for discussion see Hendry, 2005; 2010a). There is no role for caloric in modern chemistry and physics, so the temptation is to airbrush it from Lavoisier's *curriculum vitae*. This temptation ought clearly to be resisted if one wishes to understand chemistry in relationship to its past.

[13] It is possible (both logically and metaphysically) that chemistry could have come to conceive of substances in some quite different way. But the way that chemistry in fact *does* individuate substances reflects something important about the world. This, I would argue, is one good reason to endorse microstructural essentialism.

[14] In a thought-provoking paper, Joseph Earley (2006) has also used this distinction between chemical substances and 'substances' in the metaphysical sense. My use of the term 'mode' here is not meant to invoke any particular categorial framework in ontology, but only to suggest ontological dependence.

[15] It would be better to use the term 'mixt', following Paul Needham (2006, 2009), to indicate that some historical authors, including Aristotle, do not distinguish between (what are now regarded as) compounds and homogeneous mixtures such as solutions. From the modern point of view 'mixt' is a disjunctive term.

if, *contra* Aristotle, the elements persist in the compound (and are jointly exhaustive of it) then presumably there must also be some heterogeneity, because the ferrous sulphide is partly iron and partly sulphur.[16] In any case, homogeneity is not sufficient for being a compound in modern chemistry, since solutions may be regarded as homogeneous mixtures. So the phrase 'homogeneous mixture' is not an oxymoron.

Why should we say, with the atomists and against Aristotle, that iron and sulphur live on in iron sulphide? The yellow of the sulphur and grey of the iron have after all disappeared, replaced by uniformly black stuff. For modern chemistry, the sulphur and the iron live on because the nuclei, and more specifically their nuclear charges, survive the process of combination. The extension of the terms 'sulphur' and 'iron' must here be understood as reaching beyond the free elements (e.g. rhombic sulphur and metallic iron) to include all their states of chemical combination. However, there are complications, which mean we cannot simply adopt the classical atomist picture of chemical combination, which Aristotle rejected (see Needham & Hendry, 2018). We have established that Aristotle's problem of mixture can, under certain assumptions, be regarded as a case of the SCQ. We have established that modern chemistry supports those assumptions. Does modern chemistry therefore provide an answer to the SCQ? I do not think it does, for the simple reason that it provides no sharp distinction between compounds and mixtures. There are clear cases of compounds, there are clear cases of mixtures, and there are penumbral cases, such as solutions. Notice, however, that to give an account of the distinction between substances and mixtures is to give a general account of the sameness and difference of substances, for a mixture is a body of stuff in which there is more than one substance. But if one individuates substances by their structures at the molecular scale, then one should expect the sameness and difference of substances to be a vague and multidimensional affair, because the sameness and difference of structures at the molecular scale is a vague and multidimensional affair.

So we should expect the answer to the SCQ for chemical substances to be vague and multi-dimensional. We should also expect it to involve energy, because that is how chemistry and physics answer questions about stability. A necessary condition for chemical combination to occur is that the composite is more stable than the components separately, i.e. the Gibbs free energy associated with the change should be negative. But thermodynamics tells us that some changes are 'spontaneous', in that the associated change in the Gibbs free energy is negative, but they nevertheless happen only very slowly.[17] In short, there is a distinction between thermodynamic and kinetic stability: this means that it is physically possible that some thermodynamically unstable but kinetically stable things continue to exist, in the sense that they are in the process of spontaneously transforming into something else, but are doing so only very slowly. Meanwhile we have to include their powers and susceptibilities in a general account of why things happen. Energetic stability on its own is not enough to understand the physical existence of a composite: lifetime and environment, or rather lifetime *in an environment*, must also be taken into account. In very general terms, how slowly must something be spontaneously be converting into something else in order to be said to exist? Presumably, slowly enough to be detected, and therefore slowly enough to be able to display at least some of its characteristic powers and susceptibilities.

Also closely related to the SCQ is a question that chemistry has been able to formulate precisely ever since it began closely to engage with physics, in the form of quantum mechanics, during the 1920s: when does a group of atoms form a molecule?[18] This is the third kind of compositional relationship. The question is very neatly, but I will argue incompletely, answered by comparing and contrasting the electronic energies of the dimers of hydrogen (H_2) and helium (He_2). H_2 is said to be stable because there is a net energy decrease on formation of the molecule, while for He_2 there is no such decrease. The molecule is not energetically favoured over the separated atoms, which simply drift apart. For this reason He_2 is sometimes said not to exist, but that is an incomplete account of the situation: the environment and the lifetime of the species must be taken into account. Helium atoms interact weakly via van der Waals forces: random variations in the electronic charge distribution give rise to a dipole on one atom, which induces dipoles in its neighbours. The resulting attractive forces are very weak, but at very low temperatures a significant proportion of helium exists as dimers, significantly altering the behaviour of liquid helium near absolute zero. Now the very same interactions take place at higher temperatures, it is just that they are far too weak to constrain the motions of atoms. One might say that helium dimers come into fleeting existence only for thermal energy (in the form of vibrations) to rip them apart, but that fails to distinguish the low-temperature and the room-temperature situations. At room temperature the translational kinetic energy of the helium atoms overwhelms the van der Waals attraction. When two helium atoms collide nothing holds them together. The dimer doesn't vibrate because the 'restoring force' is too weak to bring the two atoms back from the recoil even once. The shallow local van der Waals minimum in the potential energy surface is merely a bump on the road passed over during the collision. It does not constrain the motion of the individual helium atoms. The two atoms neither move as a composite object nor form a system with any composite motions. That's why there is no virtue in seeing them as a dimer. At low temperatures the powers and susceptibilities of He_2 must be taken into account when describing the behaviour of helium, but this is not the case at higher temperatures. At room temperature there is no He_2, which is why its powers and susceptibilities need not be taken into account in understanding the behaviour of room-temperature helium.

An interesting penumbral case is provided by reactive intermediates: do they have a distinct existence, or are they just transition stages between genuine existents? When chemical reactions occur, the reactants very often have to pass through a higher-energy transition state before the reaction can proceed. This provides an energetic barrier to the reaction the height of which (the activation energy) partly determines how fast the reaction occurs (hence this is also the basis of the distinction between thermodynamic and kinetic stability). But at the top of this energetic 'hill' there may be a little hollow, or dip. Depending on the depth of this dip, and the energetic environment, a particular group of atoms may occupy it for some considerable time. In some cases, the intermediate may even be isolable (see Fig. 7).

From an energetic point of view alone, the difference between the two cases is a matter of degree, even though important distinctions hang on it:

> For a reaction proceeding through the *intermediate*, there is a 'dip' or minimum in the energy profile diagram. The deeper the dip, the

[16] This we know anyway, if matter is discontinuous, as modern chemistry and physics presume.

[17] One of these is the conversion of diamond into graphite.

[18] Strictly speaking, it is a version of the SCQ only on the assumption that atoms continue to exist in a molecule. This may seem a substantial assumption, but the Atoms in Molecules (AIM) programme provides a quantum-mechanically non-arbitrary way to 'carve up' a molecule exhaustively into neutral atoms (Bader, 1990; Popelier, 2000, Chapter 3). Atoms in molecules are not spherical, but free atoms are not always spherical, and it is highly implausible in any case that sphericity should be an *essential* property of an atom.

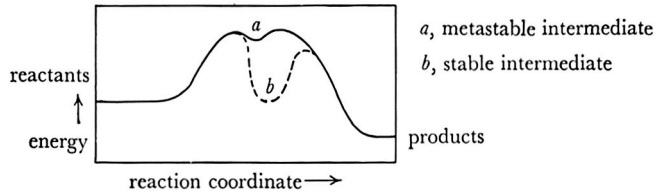

Fig. 7. Energy profiles for reactions proceeding through intermediates, from Gould, 1959, p. 130.

> more stable the intermediate and the more sure we may be of its existence. ... In the extreme case the dip becomes so slight that the intermediate *a* is experimentally indistinguishable from a transition state. If the intermediate is isolable, we are in effect considering two reactions, each with its own transition state. In such cases, a substance becomes designated as an intermediate simply because the 'reaction' originally chosen is a composite one. (Gould, 1959, 130)[19]

Crucially, even if the dip is not deep enough for the intermediate to be isolated it might be detected directly, because it exists long enough to go through a few cycles of some characteristic vibration, and so in principle be detectable by spectroscopic means. Despite being too unstable for separation, it demonstrates its own existence by exercising its powers.[20] Conversely, if the dip is too shallow the intermediate cannot make its existence known in this way. Once again, this suggests that we cannot understand molecular existence in terms of energy alone. We also need to know about timescales.

For these reasons I must regard as incomplete the 'bound-state proposal' recently advanced as a response to the SCQ by Kerry McKenzie and F.A. Muller:

> *[Physical] objects form a composite object iff these physical objects interact and are in a common bound state*, where '*common* bound state' means that the composing objects are in the potential well that results of their mutual physical interaction. (2017, 234)

This proposal seems to have a number of virtues.[21] Firstly, although the condition applies widely, it is technically a 'moderate' one in van Inwagen's terms because it entails neither mereological universalism nor mereological nihilism. Secondly, it aligns composition with physical explanation. As we have seen, chemists and physicists typically explain the existence of various objects in terms of relationships between energy and structure. A group of objects being in such a common bound state is (at least sometimes) the explanation of why they do not 'fly apart' (2017, 235).

However, the reference to a 'potential well' is less clear than it sounds. Does it mean the global minimum on a potential energy surface for the relevant parts, or a local one? If a global minimum is required the bound-state proposal doesn't deal well with composite objects whose existence over time results from their being metastable (see above): physical systems that are unstable with respect to close-lying structures, but which persist for relatively long periods owing to the slow rate of conversion. These include glasses, which might be regarded as very slowly relaxing into crystalline states, but also diamonds (because graphite is a lower-energy configuration of carbon atoms), and chemical elements other than iron (because iron represents the global minimum on a graph of binding energy per nucleon). Philosophers often like to embrace the counterintuitive consequences of their theories, but surely the cost here is too high. Hence 'minimum' should be interpreted as 'local minimum,' in which case 'potential well' means (a small region around) a turning point at which the curvature of the graph of energy as a function of geometrical configuration is positive. There are many more such points than one might imagine: take the rotation of the CH_3-group 'propellors' around the carbon-carbon bond in ethane, discussed earlier. Interference between the hydrogen atoms presents a barrier to rotation, so the 'eclipsed' conformation is of slightly higher energy than the 'staggered' conformation. In rotating, the ethane molecule therefore traverses a sinusoidal potential energy curve, inhabiting the troughs for a 'finite, but very short *residence time*' (Bassindale, 1984, p. 51). Does a series of staggered ethane molecules pass into and out of existence millions of times a second? Under my earlier proposal, according to which structure is a creature of abstraction, this is less troubling than it sounds because the ethane molecule itself survives these changes. The situation with helium molecules is worse: the two atoms instantaneously experience an attraction (such a romantic tale), momentarily occupying a common potential well before flying apart on the rebound. The bound-state proposal as formulated forces us to bite the bullet and say that two helium atoms colliding form a fleeting molecule. Defending the bound-state proposal, one might say that we tend to ignore fleeting existences because they don't make themselves felt, but this is like the mereological universalist, who is forced to invoke pragmatic considerations to explain why the Eiffel Tower and my left big toe do not form a composite object whose existence is as kosher as that of a hydrogen molecule. I think it is better to amend the metaphysics than to invoke such wide-ranging pragmatic corrections. The problem is really (as we saw earlier) that the low-temperature and room-temperature situations need to be treated differently.

In that spirit I suggest two friendly amendments to McKenzie and Muller's proposal. Firstly, to avoid the unwanted room-temperature helium molecules, one might say that a composite object exists when its parts *are trapped* in a potential well, in that they are in the potential well and have insufficient kinetic energy to escape. There are modal and temporal aspects to the difference between helium at low temperature and at room temperature. At low temperature the interaction between the atoms is strong enough to pull the atoms back from their thermal vibrations, and the dimer lives long enough to display its characteristic powers and susceptibilities, which include vibrating at specific frequencies. Neither of these things is true at room temperature. The modal aspect is suggested by the name McKenzie and Muller chose for their proposal, but gets lost in their articulation of it. My second suggested amendment is to restrict the scope of their proposal because I am less confident than McKenzie and Muller that it accounts for the existence of animals: 'if the particles of a cat, say, were not in a bound state they would fly apart in all directions' (2017, 235). It is not so obvious that the particles in a cat (a far-from-equilibrium system) are *not* flying apart, since it is continuously shedding matter in various directions. Yet the cat exists nonetheless (as a process), suggesting that we should look elsewhere for a physical explanation of its existence. The best one can hope for McKenzie and Muller's proposal, even an amended version of it, is as a disjunct in what van Inwagen (1990, 64–71) calls 'series-style' responses to the SCQ. It is not at all surprising to me that cats and molecules should bear quite different relationships to their material parts.

5. Conclusion: structure, scale and emergence

I began this paper with an extended complaint about how, when they discuss structure and composition, philosophers often misuse the word 'arrangement'. The main mistake they make is to assume that composed things are really nothing but arrangements of their parts. If an 'arrangement' is just a static array then it is indeed hard to see how the parts arranged this way are really any different from the same parts

[19] Note that although Gould puts the word 'reaction' in inverted commas, there is no logical difficulty in a chemical reaction being composite in the sense he discusses. Many well-known chemical reactions are composite in this way.

[20] This is why it is sometimes possible to create and detect a nucleus of a superheavy element whose existence is too fleeting for it to count as a true chemical element: it can be detected spectroscopically but cannot (physically) live long enough to capture electrons and have them relax into a stable electronic configuration. See Hendry, 2020.

[21] I am not sure that their proposal is meant entirely seriously (see McKenzie & Muller, 2017, 241), so I hope they will forgive my po-faced response.

arranged some other way. This is why, I think, compositional nihilism is so bafflingly popular among those who try to address the SCQ. Being arranged in some particular way cannot, surely, add anything to the situation. But that is a poor model for composition in the physical sciences. Nothing like 'arrangements' of this kind appear in the explanations offered by sciences that study chemical substances and their structures at the molecular scale. Nuclei and electrons are always in motion. Experiments reveal different structures at different scales of energy, time and length. This is perhaps less surprising than it might seem if we consider how structure and energy are related: structure is what gets 'frozen in' when matter no longer has enough energy to escape from the attractive forces that tend to confine it. Whole new realms of possibility come into being when we turn down the energy dial far enough for nuclei to capture electrons in the structured entities we call atoms and molecules. From this condensation emerges a great diversity of structures which chemistry, crystallography and condensed matter physics characterise using two kinds of interatomic relationship: geometry and the chemical bond. One might conclude that substances, and the structures that characterise them, are emergent. Clearly, substances are dependent on their structures at the molecular scale, which are in turn dependent on the entities, properties and relations of which they are formed (see Hendry, 2017, 2019). Yet we have seen that a physical system may present different structures at different scales. Since there is no general reason to think that the structures we find at lower energy scales, or at longer time or length scales, are reducible to those we find at higher energies etc., one might say that structure emerges from the motions of physical systems, and that different structures emerge at different scales. I think that this is an interesting and significant insight, with two aspects. One is anodyne: new things come into being under different conditions. The other is less anodyne: existence is tied to lifetime, and what exists at one scale, and is thereby detectable by one experimental method, need not exist at another scale, and so may be invisible to experimental methods at that other scale. This might seem perspectival, but as already noted these are matters of physical interaction, not of perception or conception.

Now scientists and philosophers sometimes say that arguments like these are much less significant than they sound. They support such claims in different ways. Some turn away from emergence because they find it unclear. This is a pity I believe, because the various versions of emergentism are no less intelligible or able to confer enlightenment than the spectrum of reductionist ideas to which they are opposed. Scientists sometimes say that even though it is not possible to derive chemical explanations from fundamental physics something can be both emergent and 'reducible in principle', and moreover that we have good reasons to believe that everything is reducible in principle: a fully completed physics would account for everything that science can know. Steven Weinberg (2001, Chapter 10) quite explicitly makes a distinction of this sort, between reductionism as a 'research programme' and as a 'world view'.[22] The important thing to see is that when Weinberg says that 'in principle' fundamental physics explains everything, even if not in practice, he must mean something like the following: there is an unknown future physical theory that, when applied to the whole world, produces an equation that nobody could write down. This equation 'explains' every contingent fact (or a large proportion of them) that can broadly be expressed in the language of physics, despite the fact that there is no reason at all to think that this equation could be solved by any finite intelligence even if it were to be given very large (though still finite) computing resources. This, I would suggest, is a Pickwickian sense of 'explains'. Philosophers sometimes say that the emergence I have argued for can only be of a so-called 'weak' sort. 'Strong' emergence would require the emergents to have causal efficacy over and above the things on which they depend, but exclusion arguments exclude that possibility. Against these scientists and philosophers I say the following. Claims of 'reducibility in principle' require scientific support: a systematic grounding in the actual performance of real scientific theories. Exclusion arguments depend on strong assumptions about the causal (or dynamical) completeness of physics.[23] Given the scientific evidence, there is no reason why the completeness of physics should be regarded as a constraint on naturalistic discussions of the ontology of the physical world. In the meantime I feel free to proceed without this constraint, just as the atheist should feel free to address questions about what there is, where it has come from and how one should live, free of any assumption of a personal and transcendent creator, without being able to demonstrate the non-existence of that creator.

[22] For an eloquent and explicit rejection of 'reducibility in principle' by physicists see Laughlin & Pines, 2000.

[23] Perhaps surprisingly, very few scientists or philosophers feel the need to argue for such completeness claims explicitly. For a response to two arguments from the literature see Hendry, 2010b.

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